

Floating Phase in 1D Transverse ANNNI Model

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To study the ground state of ANNNI chain under transverse field as a function of frustration parameter κ and field strength Γ , we present here two different perturbative analyses. In one, we consider the (known) ground state at $\kappa = 0.5$ and $\Gamma = 0$ as the unperturbed state and treat an increase of the field from 0 to Γ coupled with an increase of κ from 0.5 to $0.5 + r\Gamma$ as perturbation. The first order perturbation correction to eigenvalue can be calculated exactly and we could conclude that there are only two phase transition lines emanating from the point $\kappa = 0.5$, $\Gamma = 0$. In the second perturbation scheme, we consider the number of domains of length 1 as the perturbation and obtain the zero-th order eigenfunction for the perturbed ground state. From the longitudinal spin-spin correlation, we conclude that floating phase exists for small values of transverse field over the entire region intermediate between the ferromagnetic phase and antiphase.

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I. INTRODUCTION

The transverse Axial Next-Nearest Neighbour Ising (ANNNI) model is one of the simplest Ising models that contains tunable frustration and tunable quantum fluctuation. In one dimension, it is defined (for spin= $\frac{1}{2}$) by the Hamiltonian [1]

$$\mathcal{H} = -J \sum_{j=1}^N (s_j^z s_{j+1}^z - \kappa s_j^z s_{j+2}^z) - \Gamma \sum_{j=1}^N s_j^x \quad (1)$$

Here the first term describes a ferromagnetic nearest-neighbour interaction of strength $J(>0)$ between longitudinal components of spin $s^z (= \pm 1)$, the second term describes an antiferromagnetic second neighbour interaction of strength κJ also in the longitudinal direction, and the third term describes an external field in the transverse direction of strength Γ . The ratio $\kappa (>0)$ is called the frustration parameter. This Hamiltonian describes a classical ANNNI chain subjected to a transverse field as well as a transverse (nearest-neighbour) Ising model with an additional frustrated second nearest-neighbour interaction. In this paper, we shall deal with the *ground state* (zero-temperature) phase diagram of the Hamiltonian \mathcal{H} . It is known [1, 2] that for $\kappa = 0$ (only nearest-neighbour interaction), there is a ferromagnetic to paramagnetic second order phase transition at $\Gamma = J$. On the other hand, for $\Gamma = 0$ (classical ANNNI chain) [1, 3] the ground state is ferromagnetic for $\kappa < 0.5$ and antiphase (+ + -- type) for $\kappa > 0.5$, with a ‘multiphase point’ at $\kappa = 0.5$. At the multiphase point [3] the ground-state has very high ($\sim g^N$, where g is the golden ratio $(\sqrt{5} + 1)/2$) degeneracy as any combination of antiphase and ferromagnetic patches will serve as ground state configuration. From approximate analytic and numerical approaches [1, 4], early studies had proposed a phase diagram (Fig. 1) that consists of ferromagnetic,

paramagnetic and antiphase regions, alongwith a region of what is called *floating phase*. The n^{th} neighbour spin-spin correlation function in the longitudinal direction

$$C^z(n) \equiv \langle s_j^z s_{j+n}^z \rangle - \langle s_j^z \rangle^2 \quad (2)$$

decays exponentially with distance in the ferromagnetic, antiphase and paramagnetic regions but decays algebraically in the floating phase. The evidence for the presence of floating phase is provided by quantum Monte Carlo simulation [5] and by exact numerical diagonalisation of small systems [4, 6], one of which [4] extends even upto a length of 32.

Recently, a question has arisen on the existence of the floating phase, as a recent study [7] has claimed that the floating phase exists only within a strip of infinitesimally small width. The transverse ANNNI chain is related to the two-dimensional classical ANNNI model by Suzuki-Trotter transformation. The phase diagram for this model is also similar to Fig. 1 (with Γ replaced by temperature). Here also the earlier studies [3] support the existence of floating phase in view of Monte Carlo simulations by Selke and others [8] and approximate analytic calculations by Villain and Bak [9], while a recent measurement of dynamical exponent [10] and a density matrix renormalisation group analysis [11] claim that the floating phase exists, if at all, along a line only. We have also studied [12] some static and dynamical properties of the 2D ANNNI model by Monte Carlo simulation. Our study also indicates that the floating phase exists, if at all, only along a line. The question is to whether the floating phase exists only along a line or extends over a region in the case of transverse ANNNI chain is the basic motivation of this paper.

In this paper we perform two perturbation calculations with an aim to have an idea about the phase that exists near the multiphase point for non-zero transverse field. Our conclusion is that there exists floating phase over a

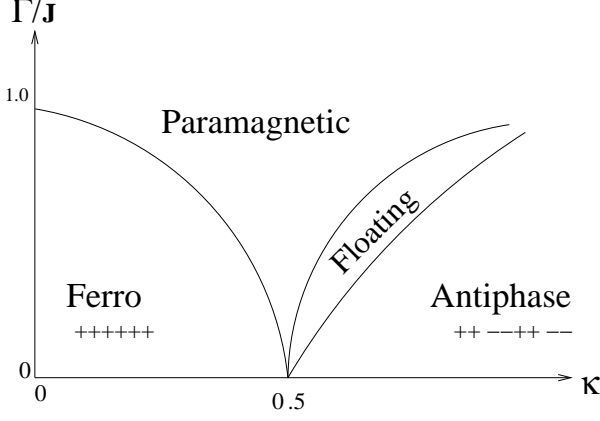


FIG. 1:

Schematic phase diagram of the transverse ANNNI model according to early investigations [1,2].

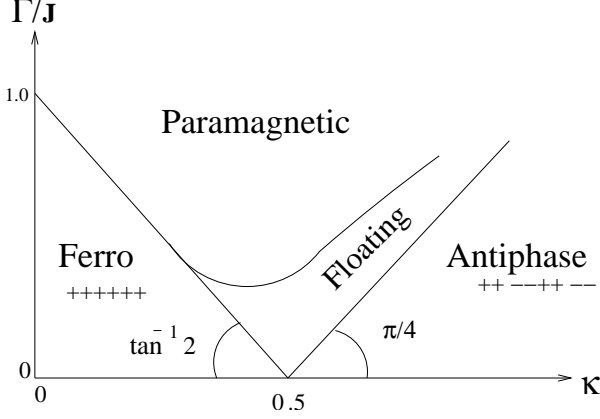


FIG. 2:

Schematic phase diagram of the transverse ANNNI model according to the present work.

region extending from ferromagnetic phase to antiphase (for small values of Γ) and the phase diagram looks like Fig. 2. This result is in contradiction with previous results as none of the previous studies had predicted floating phase for $\kappa < 0.5$. We must mention that all our results are true only at “small” values of Γ and the quantitative details of this diagram is not reliable at $\Gamma \sim 1$. However, the topological structure of the diagram should be correct. This article is organised as follows. In Sections II and III, the first and the second perturbation schemes will be presented (respectively) and we shall conclude with some discussions in Sec. IV.

II. THE FIRST PERTURBATION SCHEME

A. Principle

We shall now present a first order perturbation calculation around $\kappa = 0.5$ by rewriting the Hamiltonian \mathcal{H} of

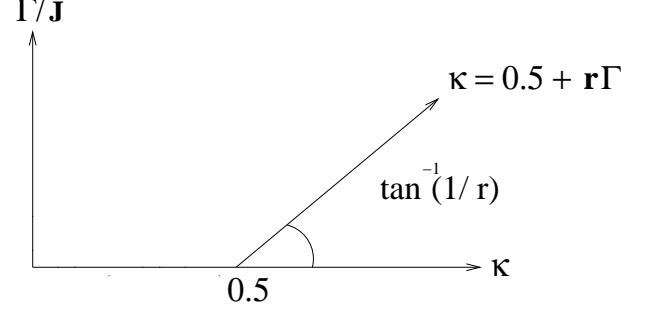


FIG. 3:

Scheme of the first perturbation treatment. The transverse field is altered from 0 to a (small) value Γ and the frustration parameter κ is altered from 0.5 to $0.5 + r\Gamma$. The parameter r may vary from $-\infty$ to ∞ .

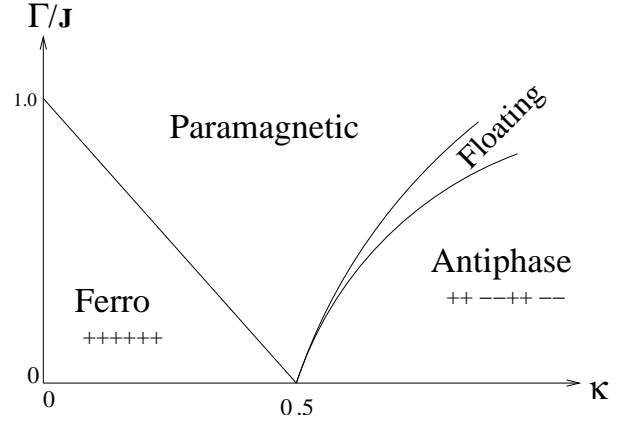


FIG. 4:

One possible type of phase diagram of the transverse ANNNI model.

Eq. (1) as

$$\mathcal{H} = \mathcal{H}_{cl} + \mathcal{H}_p$$

where

$$\mathcal{H}_{cl} = -J \sum_j [s_j^z s_{j+1}^z - \frac{1}{2} s_j^z s_{j+2}^z] \quad (3)$$

and

$$\mathcal{H}_p = \sum_j \Gamma [-s_j^x + r s_j^z s_{j+2}^z] \quad (4)$$

with $r = J(\kappa - 0.5)/\Gamma$. We always take Γ to be positive, so that negative values of r imply $\kappa < 0.5$.

We shall treat the \mathcal{H}_p as a perturbation over \mathcal{H}_{cl} . Obviously, \mathcal{H}_{cl} is the longitudinal (classical) part of \mathcal{H} at $\kappa = 0.5$ and \mathcal{H}_p includes the transverse part and an increase of κ (from 0.5) by an amount $r\Gamma$. One must note that for a perturbative treatment Γ has to be small but r need not be so. In the (κ, Γ) phase space, the perturbation takes us from the multiphase point $(0.5, 0)$ to a point $(0.5 + r\Gamma, \Gamma)$. As r varies from $-\infty$ to

∞ , the perturbation takes us from the ferromagnetic to the antiphase region (Fig. 3). The first order correction ($E^{(1)}$) to ground state energy can be calculated *exactly*. This quantity is studied as a function of r , because if there is a non-analyticity at $r = r_0$, then there will be a phase transition line emanating from the $(0.5, 0)$ point at an angle $\tan^{-1}(1/r_0)$ with the increasing κ direction. It is found that $E^{(1)}$ as a function of r is non-analytic only at $r = -0.5$ and 1 . Therefore, only two lines of phase transition meet at the multiphase point. This implies either that the floating-paramagnetic transition line touches tangentially the floating-antiphase line at this point (Fig. 4) or that the floating phase extends over the entire region from antiphase to ferromagnetic region (Fig. 2). It will be shown that a study of susceptibility and mass-gap rules out the possibility of Fig. 4 and points to the validity of Fig. 2. Thus, the final conclusion from the first perturbation scheme is that the boundary between the ferromagnetic (antiphase) and the floating phase emanates from the multiphase point at an angle $\tan^{-1} -2 (\tan^{-1} 1)$ with the κ axis. The second perturbation scheme also supports this conclusion and additionally enables us to obtain an approximate phase diagram. We shall now transform our problem to a certain problem for the nearest neighbour transverse Ising model and then through a study of the nearest neighbour model, obtain the expression for $E^{(1)}$.

B. Transformation to Nearest-neighbour Model

We start by noting that at $\kappa = 0.5$ (the ‘multiphase point’ [3]) the ground state of \mathcal{H}_{cl} , the unperturbed Hamiltonian, is a highly degenerate state and any spin configuration that has no spin-domain of length unity (i.e. no $++-++$ or $--+-$ type arrangement) can be the ground state. The number of domain walls is immaterial and can be anything between 0 and $N/2$, N being the total number of spins. (Of course, for periodic boundary there can be only an even number of walls.) Let us denote the set of all such configurations as \mathcal{S} . Also, let the population of this set be ν which incidentally is of the order of g^N as mentioned in Sec. I [3]. Now, the first-order correction to the eigenvalue are the eigenvalues of the $\nu \times \nu$ matrix P , whose elements are

$$P_{\alpha\beta} \equiv \langle \alpha | \mathcal{H}_p | \beta \rangle$$

where $|\alpha\rangle$ and $|\beta\rangle$ are configurations within \mathcal{S} . The matrix P can be easily given a block diagonal structure. Note that $s_j^x |\beta\rangle \in \mathcal{S}$ if and only if the j -th spin lies at the *boundary* of a domain, and the domain too has length larger than 2. Also, in such a case, s_j^x operating on $|\beta\rangle$ will translate the wall at the left (right) of the j -th site by one lattice spacing to the right (left). This immediately leads us to the important conclusion that $P_{\alpha\beta} \neq 0$ if and only if $|\alpha\rangle$ and $|\beta\rangle$ have equal number of domain walls. Thus, we can break up \mathcal{S} into subsets $\mathcal{S}(W)$, where $\mathcal{S}(W)$ contains all possible spin distributions with W walls (W

$= 2, 4, \dots, N/2$). Now, the $\nu \times \nu$ matrix P gets block-diagonalised into matrices of size $\nu_W \times \nu_W$,

$$P_{\alpha\beta}(W) \equiv \langle \alpha | \mathcal{H}_p | \beta \rangle \quad (5)$$

where ν_W is the population of $\mathcal{S}(W)$ and $|\alpha\rangle, |\beta\rangle \in \mathcal{S}(W)$. We now observe that the longitudinal term in \mathcal{H}_p only contributes a diagonal term $r\Gamma(N - 4W)$ to $P_{\alpha\beta}(W)$, so that one can write

$$P(W) = M(W) + r\Gamma(N - 4W)\mathbf{1}. \quad (6)$$

Here $\mathbf{1}$ is the $\nu_W \times \nu_W$ unit matrix, $M_{\alpha\beta}(W) \equiv \langle \alpha | \mathcal{H}_q | \beta \rangle$ and $\mathcal{H}_q = -\Gamma \sum_j s_j^x$ is the transverse part of \mathcal{H}_p . Thus the non-trivial problem is to solve the eigenproblem of $M(W)$.

To proceed with the matrices $M(W)$, let us construct from each member $|\alpha\rangle$ of $\mathcal{S}(W)$ a configuration $|\alpha'\rangle$ by removing one spin from each domain. The total number of spins in $|\alpha'\rangle$ will obviously be $N - W = N'$, say. Such a transformation was also used by Villain and Bak [9] for the case of two-dimensional ANNNI model. The set $\mathcal{S}'(W)$ composed of the states $|\alpha'\rangle$ is then nothing but the set of all possible distributions of N' spins with W walls, with no restriction on the domains of length unity. It is easily seen that the matrix

$$M'_{\alpha\beta}(W) \equiv \langle \alpha' | \mathcal{H}_q | \beta' \rangle$$

will then be identical with $M(W)$ since the element

$$\langle \alpha' | \sum_{j=1}^{N'} s_j^x | \beta' \rangle$$

is non-zero when and only when

$$\langle \alpha | \sum_{j=1}^N s_j^x | \beta \rangle$$

is non-zero. The eigenproblem of $M'(W)$ becomes simple once we observe that $\mathcal{S}'(W)$ is nothing but the set of degenerate eigenstates of the Hamiltonian

$$\mathcal{H}'_0 = -J \sum_{j=1}^{N'} s_j^z s_{j+1}^z$$

corresponding to the eigenvalue

$$E_W = -J(N' - 2W). \quad (7)$$

Thus, if we perturb \mathcal{H}'_0 by \mathcal{H}_q , then the first-order perturbation matrix will assume a block diagonal form made up of the matrices $M'(W)$ for all possible values of W .

C. Study of the Nearest-neighbour Model and Further Analysis

To solve the perturbation problem for $\mathcal{H}'_0 + \mathcal{H}_q$, we note that this Hamiltonian is the same as \mathcal{H} of Eq. (1)

with $\kappa = 0$, namely,

$$\mathcal{H}^{TI} = - \sum_{j=1}^{N'} [J s_j^z s_{j+1}^z + \Gamma s_j^x].$$

This is the Hamiltonian for the standard transverse Ising model. The exact solution for this Hamiltonian is readily available [2, 13, 14]. The exact expression for the energy eigenstates are (for periodic chain in the thermodynamic limit [15]),

$$E = 2\Gamma \sum_k \xi_k \Lambda_k \quad (8)$$

where ξ_k may be 0, ± 1 and k runs over $N'/2$ equispaced values in the interval 0 to π . Also, Λ_k stands for $\sqrt{(\lambda^2 + 2\lambda \cos k + 1)}$, where λ is the ratio J/Γ . For $\Gamma = 0$, the energy E must be the same as E_W of Eq.(7), so that

$$2 \sum_{k=0}^{\pi} \xi_k = -(N' - 2W). \quad (9)$$

Clearly, the different values of the quantity

$$\left(\frac{\partial E}{\partial \Gamma} \right)_{\Gamma=0} = 2 \sum_{k=0}^{\pi} \xi_k \cos k$$

correspond to the first order perturbation corrections to the different levels. They are therefore also the eigenvalues of the M' matrix. Thus the eigenvalues of the matrix $P(W)$ of Eq.(6) are

$$E_P = r\Gamma(N - 4W) + 2\Gamma \sum_{k=0}^{\pi} \xi_k \cos k \quad (10)$$

Keeping N fixed we have to find, for which value of W and for which distribution of ξ_k , E_P is minimum subject to the constraint (9). For a given value of $\sum \xi_k$, this minimisation is achieved if -1 values of ξ_k accumulate near $k = 0$ and +1 values near $k = \pi$. Let the desired distribution be

$$\xi_k = \begin{cases} -1 & \text{for } k = 0 \text{ to } \theta \\ 0 & \text{for } k = \theta \text{ to } \phi \\ 1 & \text{for } k = \phi \text{ to } \pi \end{cases} \quad (11)$$

Eq.(9) now gives

$$N/N' = (4\pi - \theta - \phi)/2\pi \quad (12)$$

and one obtains,

$$E_P = - \frac{N\Gamma}{4\pi - \theta - \phi} [r(4\pi - 3\theta - 3\phi) + 2(\sin \theta + \sin \phi)]$$

This quantity attains a minimum value only when θ and ϕ are equal and their common value (ϕ_0 , say) satisfies the condition

$$2\pi r = \sin \phi_0 + (2\pi - \phi_0) \cos \phi_0, \quad (13)$$

The minimum value of E_P is given by,

$$E^{(1)} = -N\Gamma[3r - 2 \cos \phi_0]. \quad (14)$$

This is the exact expression for the first order perturbation correction to ground state energy. It is easily seen that for $r < -0.5$, that is, for $\Gamma/J < (1 - 2\kappa)$, one has $\phi_0 = \pi$ and $W = 0$ (ferromagnetic phase), while for $r > 1$, that is $\Gamma/J < (\kappa - 0.5)$, one has $\phi_0 = 0$ and $W = N/2$ (antiphase). As r varies from -0.5 to 1 , ϕ_0 gradually changes from π to 0 according to Eq.(13). The second derivative of $E^{(1)}$ with respect to r blows up at $r = -0.5$ and 1 , indicating two critical lines there. One can see from Eq. (13) that except for these two values, r is an analytic function of ϕ_0 and hence, by Eq. (14), $E^{(1)}$ is also an analytic function of r . We have also checked explicitly (Appendix A) that no higher derivative of $E^{(1)}$ with respect to r blows up at any other value of r .

As mentioned in Sec. IIA, we can now conclude that the phase diagram is either like Fig. 2 or like Fig. 4.

D. Study of Longitudinal Susceptibility

We shall now show that an analysis of longitudinal susceptibility points to the possibility of Fig. 2, rather than of Fig. 4.

Let us call the eigenstate of $\mathcal{H}'_0 + \mathcal{H}_q$ corresponding to $\theta = \phi = \phi_0$ as $|\psi'\rangle$. This state will be composed of the spin-distributions that belong to $\mathcal{S}'(W)$ and can be written as

$$|\psi'\rangle = \sum_{j'} a_{j'} |j'\rangle$$

where $|j'\rangle$ runs over all the states in $\mathcal{S}'(W)$. If we construct from each state $|j'\rangle$ another state $|j\rangle$ by adding one spin to each domain, and then combine these states with the same coefficients, then we arrive at a state $\sum_j a_j |j\rangle$ where $a_j = a_{j'}$. This is an eigenstate of $M(W)$ and hence of $P(W)$ (see Eq. (6)) and this eigenstate is nothing but the zero-th order eigenfunction $|\psi^{(0)}\rangle$ for the perturbed ground state of $\mathcal{H}_{cl} + \mathcal{H}_p$. One should observe that although the spin-spin correlation may not be equal for $|j\rangle$ and $|j'\rangle$, the longitudinal magnetisation M_z must be the same for them (- equal number of positive and negative spins are added while transforming $|j\rangle$ to $|j'\rangle$). Thus, the longitudinal susceptibility

$$\chi_z \propto \langle M_z^2 \rangle - \langle M_z \rangle^2$$

of $|\psi^{(0)}\rangle$ must be the same as that of $|\psi'\rangle$. The spin-spin correlation

$$C^z(n) \equiv \langle s_i^z s_{i+n}^z \rangle$$

for $|\psi'\rangle$ may be calculated (see Appendix B). In the case of $\Gamma < J$, for the entire range $0 < \phi_0 < \pi$, the correlation is

$$C^z(n) = A \frac{1}{\sqrt{n}} \cos[n(\pi - \phi_0)]$$

where A is a constant. This is clearly a floating phase. The susceptibility χ_z is hence infinity for both the states $|\psi'\rangle$ and $|\psi^{(0)}\rangle$. This leads us to the conclusion that the zero-th order eigenstate is in floating phase and hence, at least for small values of Γ , the ground state of transverse ANNNI chain must be a floating phase for all values of r between -0.5 and 1 . Of course, for large values of Γ the perturbation corrections may cancel the divergence of susceptibility and lead to a paramagnetic state.

One must note that it is difficult to derive an *exact* relationship between the correlation in state $|\psi^{(0)}\rangle$ and the same in state $|\psi'\rangle$. Although a similar relationship was obtained by Villain and Bak [9], we do not extend that derivation here. It is interesting to note that Villain and Bak (and also Uimin and Rieger [4]) assumed the wave number to be equal to the number of domain walls per site, but we shall soon find that this conclusion disagrees with the results obtained from our second perturbation scheme.

E. Study of Mass Gap

We shall now show that an analysis of mass gap also points to the possibility of Fig. 2, rather than of Fig. 4, thus agreeing with the conclusion from the analysis of longitudinal susceptibility.

One signature of floating phase or diverging correlation length is vanishing *mass-gap* [2, 16]. Let us now study the first order (in Γ) correction to the mass-gap. Since the first order correction to all energy states is given by the different possible values of E_P of Eq. (10), the correction to the energy of the first excited state is the smallest possible value of E_P apart from the ground state $E^{(1)}$. To find the lowest excitation over the ground state, we note that such excitation is possible either (i) by keeping $\sum \xi_k$ fixed and rearranging the ξ_k values; or (ii) by altering θ and ϕ and thus altering $\sum \xi_k$. For (i) the lowest excitation will correspond to an interchange of $+1$ and -1 at $k = \phi_0$, which will lead to a mass gap (for the whole system, not per site)

$$\Delta^{(1)} = \frac{8\pi\Gamma\lambda \sin \phi_0}{N'\Lambda_{\phi_0}}.$$

For (ii) the mass gap is :

$$\Delta^{(1)} = \frac{1}{2} \left(\frac{\partial^2 E_P}{\partial \theta^2} \right)_{\theta=\phi_0} (\delta\theta)^2$$

Here $\delta\theta$ is the smallest possible deviation in θ at ϕ_0 . As the smallest possible change in W , and hence in N' is 2, Eq.(12) (with $\theta = \phi$) tells us that

$$\delta\theta = \frac{2(2\pi - \theta)^2}{\pi N} \sim \frac{1}{N}.$$

This shows that for both the mechanisms (i) and (ii), the mass gap $\Delta^{(1)}$ vanishes as $N \rightarrow \infty$ for all values of

ϕ_0 between 0 and π . This shows that for all values of r between -0.5 and 1 there must be floating phase for small Γ .

For transverse Ising model ($\kappa = 0$) the phase transition occurs at $\Gamma = J$ and at $\Gamma = J + \epsilon$ the first order (in ϵ) correction to the mass gap is just Γ , and is thus nonvanishing, indicating that the divergent correlation length does not extend beyond $\Gamma = J$.

III. THE SECOND PERTURBATION SCHEME

A. Principle

In the previous section we have found that the phase diagram looks like Fig. 2. In order to reconfirm this result explicitly, we have to know the eigenfunction with first- or even zero-th order correction. As it is difficult to calculate the eigenfunction for the perturbation scheme discussed above in Sec. II, we shall perform the second set of perturbation calculation now.

Let us write the Hamiltonian \mathcal{H} of Eq. (1) for $\kappa < 0.5$ as

$$\mathcal{H} = N(h_0 + h_1 - J\kappa) \quad (15)$$

with

$$h_0 = -(1 - 2\kappa)J \frac{1}{N} \sum_j s_j^z s_{j+1}^z - \Gamma \frac{1}{N} \sum_j s_j^x \quad (16)$$

and

$$h_1 = \kappa J \frac{1}{N} \sum_j (1 - s_j^z s_{j+1}^z)(1 - s_{j+1}^z s_{j+2}^z). \quad (17)$$

Clearly, h_0 represents the Hamiltonian of standard transverse Ising model with nearest-neighbour interaction and h_1 represents the number of domains of length 1. We shall treat the operator h_1 as perturbation on the Hamiltonian h_0 . All the eigenstates of h_0 are precisely known [14] and for each eigenstate one can readily calculate the expectation value of $h_0 + h_1$ and identify the eigenstate for which $\langle h_0 + h_1 \rangle$ is the lowest. This state is the eigenstate with zero-th order perturbation correction. Therefore, the basic idea is to identify the ground state upto first order perturbation correction to eigenvalue. We carry on this scheme for all values of κ (< 0.5) and Γ and in each case calculate the correlation function (as defined in Eq. (2)) and characterise the phase therefrom.

Indeed, our results are reliable only for small values of $\langle h_1 \rangle$. Hence, this quantity must be small for the low-lying eigenstates of h_0 . As mentioned already, the operator h_1 basically counts the number of domains of length 1. For $\kappa < 0.5$ the ground state of h_0 at $\Gamma = 0$ is ferromagnetic and the low-energy states may be expected to have small $\langle h_1 \rangle$ and the perturbation treatment will be justified for small values of Γ . However, for $\kappa > 0.5$,

the ground state of h_0 will be antiferromagnetic (having domains of length 1 only) and such perturbation scheme is not valid.

For $\kappa > 0.5$ one can break up \mathcal{H} as

$$\mathcal{H} = N(h'_0 + h'_1 - 0.5J) \quad (18)$$

with the unperturbed Hamiltonian defined as

$$h'_0 = (\kappa - 0.5)J \frac{1}{N} \sum_j s_j^z s_{j+2}^z - \Gamma \frac{1}{N} \sum_j s_j^x \quad (19)$$

and the perturbation as

$$h'_1 = 0.5J \frac{1}{N} \sum_j (1 - s_j^z s_{j+1}^z)(1 - s_{j+1}^z s_{j+2}^z) \quad (20)$$

The Hamiltonian h'_0 represents a chain with only next-nearest neighbour interaction and the operator h'_1 counts (as for $\kappa < 0.5$) the number of domains of length 1. The ground state of h'_0 at $\Gamma = 0$ is antiphase, and hence has $\langle h'_1 \rangle = 0$, so that the perturbation scheme is justified. Following the principle for the previous case, one can identify numerically the eigenstate (of h'_0) for which $\langle h'_0 + h'_1 \rangle$ is a minimum. From the correlation function of this state, one can characterise the phase.

The phase diagram obtained from the analysis of the present section is shown in Fig. 5. It has the following features : (i) The floating phase exists and extends from the ferromagnetic phase to the antiphase for small Γ ; thus Fig. 2 rather than Fig. 4 is the type of the phase diagram. (ii) There is a line along which transition from floating phase to paramagnetic phase takes place; this line for $\kappa < 0.5$ (obtained using Eq.(15)) continues smoothly to the same for $\kappa > 0.5$ (obtained using Eq.(18)).

We shall now present the details of the calculation for the two ranges of κ .

B. For $\kappa < 0.5$

The Hamiltonian h_0 of Eq.(16) corresponds to nearest-neighbour transverse Ising model with (ferromagnetic) interaction strength $(1 - 2\kappa)J$. Following Eq.(8), the eigenstates of this operator are

$$\langle h_0 \rangle = \Gamma \frac{1}{N/2} \sum_k \xi_k \Lambda_k \quad (21)$$

with $\Lambda_k = \sqrt{(\lambda^2 + 2\lambda \cos k + 1)}$ as in Sec. II, but $\lambda = (1 - 2\kappa)J/\Gamma$. The line corresponding to a constant value of λ is now a straight line at an angle $\tan^{-1}(2/\lambda)$ with the κ axis (Fig. 6). For each eigenstate, the n -th neighbour longitudinal correlation function (defined by Eq. (2)) can be expressed as the Toeplitz determinant [14]

$$C^z(n) = \begin{vmatrix} G_0 & G_{-1} & G_{-2} & \cdots & G_{-n+1} \\ G_1 & G_0 & G_{-1} & \cdots & G_{-n+2} \\ G_2 & G_1 & G_0 & \cdots & G_{-n+3} \\ \dots\dots\dots & & & & \\ G_{n-1} & G_{n-2} & G_{n-3} & \cdots & G_0 \end{vmatrix} \quad (22)$$

where the elements are given by

$$G_j = -\frac{2}{N} \sum_{k=0}^{\pi} \frac{\xi_k}{\Lambda_k} [\cos(kj - k) + \lambda \cos(kj)] \quad (23)$$

Here, the wave vector k runs over the $N/2$ equispaced values in the interval 0 to π and ξ_k can be 0 or ± 1 for each of the $N/2$ values of k between 0 and π .)

Now, for any eigenstate of h_0 , the expectation value of h_1 can be calculated first by rewriting it as,

$$h_1 = \kappa J \frac{1}{N} \sum_j (1 - 2s_j^z s_{j+1}^z + s_j^z s_{j+2}^z)$$

and then evaluating the first and second neighbour correlation functions using Eq.(22). The result is,

$$\langle h_1 \rangle = \kappa J [(1 - G_0)^2 - G_1 G_{-1}]. \quad (24)$$

To find which distribution of ξ_k gives the smallest value of $\langle h_0 + h_1 \rangle$, we note that G_0 will be closest to 1, when the (-1) values of ξ_k accumulate near $k = 0$ and $(+1)$ values near $k = \pi$. Although Eq.(24) does not clearly indicate that such a distribution of ξ_k will also lead to the largest values of G_1 and G_{-1} , we have verified by going through *all* the 2^N states (for $N = 12$) that indeed such a distribution leads to the lowest value of $\langle h_0 + h_1 \rangle$. We can now assume the distribution of ξ_k values to be the same as described in Eq. (11) and calculate $\langle h_0 + h_1 \rangle$ for given values of θ and ϕ . For every κ and Γ , we take a system of 1000 spins and consider all possible choices of θ , ϕ and note the values (say, θ_0 and ϕ_0) for which $\langle h_0 + h_1 \rangle$ attains a minimum. For the entire parameter range investigated in this work, we found $\theta_0 = \phi_0$. Eq.(11) now reduces to (with $\theta = \phi = \phi_0$) a distribution, namely

$$\xi_k = \begin{cases} -1 & \text{for } k = 0 \text{ to } \phi_0 \\ 1 & \text{for } k = \phi_0 \text{ to } \pi. \end{cases} \quad (25)$$

This corresponds to our approximate ground-state eigenfunction for \mathcal{H} . We have also found that for this eigenfunction, $\langle h_1 \rangle$ is non-zero. As $\langle h_1 \rangle$ is zero for all the ground state eigenfunctions at $\Gamma = 0$, we may conclude that the state we have determined as the ground state of $h_0 + h_1$, is an excited state of h_0 . In this connection, we point out that for 2D ANNNI model, it has been proved that [17] if one neglects completely the domains of length 1 (i.e. assumes $\langle h_1 \rangle$ to be zero), then one misses the floating phase, indicating that the floating phase consists of states that do *not* belong to the ground state at the $(T, \kappa) = (0, 0.5)$ point.

For every value of κ and Γ we now have determined the value of ϕ_0 and Eq.(25) therefore gives us the ground state eigenfunction. This leads to an expression for the correlation function $C^z(n)$ of Eq.(22) in the form of a determinant, an analytic expression of which has been given in Appendix B for large values of n . The final result is as follows. For $\lambda > 1$, that is, $\Gamma/J < (1 - 2\kappa)$, the value

of ϕ_0 turns out to be π , leading to a ferromagnetic phase. For $\lambda < 1$, that is, $\Gamma/J > (1 - 2\kappa)$, there are two regions. In one region $\phi_0 < \pi$ and according to Appendix B, the correlation is

$$C^z(n) = A(\phi_0) \frac{1}{\sqrt{n}}$$

indicating a floating phase with index 0.5 and no modulation. The parameter ϕ_0 varies continuously as a function of κ and Γ (Fig. 7), but this variation affects only the amplitude A . In the other region, $\phi_0 = \pi$, and the correlation is exponentially decaying, indicating a paramagnetic phase. The values of λ and ϕ_0 and the corresponding phases in different portions of the phase diagram is indicated in Fig. 8. The phase diagram thus obtained agrees with the conclusions from our first perturbation scheme and is presented in Fig. 5.

C. For $\kappa > 0.5$

The Hamiltonian h'_0 of Eq.(18) corresponds to a chain (\mathcal{C} , say) with only next-nearest neighbour interaction and can be broken into two independent transverse Ising chains (\mathcal{C}_1 and \mathcal{C}_2 , say) each having nearest-neighbour antiferromagnetic interaction. Hence, the correlation $\sum_j s_j^z s_{j+1}^z$ in \mathcal{C} will be zero and $\sum_j s_j^z s_{j+2}^z$ in \mathcal{C} will be the same as the nearest-neighbour correlation in the constituent chains \mathcal{C}_1 and \mathcal{C}_2 . (Indeed, \mathcal{C}_1 and \mathcal{C}_2 will be uncorrelated because, any configuration of \mathcal{C}_1 will couple with equal probability to two configurations of \mathcal{C}_2 , one of which can be obtained from the other by reversing all spins.) Moreover, since each of the antiferromagnetic chains can be transformed to a ferromagnetic chain (\mathcal{C}_0 , say) by simply reversing the alternate spins, the eigenstates of h'_0 in \mathcal{C} are related to the eigenstates of a nearest-neighbour ferromagnetic transverse Ising chain \mathcal{C}_0 . We have then,

$$\langle h'_0 \rangle = \Gamma \frac{1}{N/2} \sum_k \xi_k \Lambda_k \quad (26)$$

and

$$\langle h'_1 \rangle = 0.5J(1 - G_0) \quad (27)$$

with G_0 defined by Eq. (23) but now with $\lambda = (\kappa - 0.5)J/\Gamma$. As before, k runs over $N/2$ equispaced values in the interval 0 to π . The $\lambda = \text{constant}$ line is now a straight line at an angle $\tan^{-1}(1/\lambda)$ with the κ axis (Fig. 6). As in the previous subsection, we look for the eigenstate, (i.e. the ξ_k distribution) for which $\langle h'_0 + h'_1 \rangle$ will be lowest and observe that G_0 will be largest when the (-1) values of ξ_k accumulate near $k = 0$ and $(+1)$ values near $k = \pi$. Also, investigating all the states for a chain of only 12 spins, we find that the minimum value of $\langle h'_0 + h'_1 \rangle$ corresponds to the distribution with no zero values of ξ_k . Thus, assuming the distribution of Eq.

(25), we can find numerically the value of θ (say, ϕ_0) for which $\langle h'_0 + h'_1 \rangle$ will be lowest for a chain of 1000 spins. It is found that this minimum corresponds to a non-zero value of $\langle h'_1 \rangle$, indicating that as for $\kappa < 0.5$, the unperturbed state corresponding to the ground state is an excited state of h'_0 .

As in the previous subsection, we can use the expression for $C^z(n)$ mentioned in the Appendix B as the correlation in the chain \mathcal{C}_0 . The corresponding spin-spin correlation in the ANNNI chain \mathcal{C} will be

$$C_A^z(n) = \begin{cases} 0 & \text{for odd } n \\ (-1)^n C^z(n/2) & \text{for even } n \end{cases}$$

In this expression, the $(-1)^n$ factor takes account of the mapping between the ferromagnetic and antiferromagnetic chains. The final result is as follows. For $\lambda > 1$, that is, $\Gamma/J < (\kappa - 0.5)$, the value of ϕ_0 turns out to be π , so that the correlation in the chain \mathcal{C}_0 is constant and the correlation $C_A^z(n)$ corresponds to a perfect antiphase. For $\lambda < 1$, that is, $\Gamma/J > (\kappa - 0.5)$, there are two regions. In one region $\phi_0 < \pi$ and according to Appendix B, the correlation is

$$C_A^z(n) = A(\phi_0) \cos\left(\frac{n\pi}{2}\right) \frac{1}{\sqrt{n}} \quad (28)$$

indicating a floating phase with index 0.5 and modulation

$$q = \pi/2.$$

The parameter ϕ_0 varies continuously as a function of κ and Γ (Fig. 9), but this variation affects only the amplitude A . In the other region, $\phi_0 = \pi$, and the correlation in \mathcal{C}_0 is exponentially decaying, indicating a paramagnetic phase with the same modulation. The values of λ and ϕ_0 and the corresponding phases in different portions of the phase diagram is indicated in Fig. 8 and the resulting phase diagram is presented in Fig. 5, which agrees with the conclusions from our first perturbation scheme.

IV. DISCUSSION

In this section we shall point out some features of the phase diagram we have obtained.

(1) In the floating phase ($\lambda < 1$) the spin-spin correlation decays as

$$C^z(n) = A \frac{1}{n^\eta}$$

with $\eta = 0.5$. It is interesting to note that on the boundary between the floating and the ordered (ferromagnetic or antiphase) state λ is 1 and ϕ_0 is 0 or π and the correlation decays algebraically with $\eta = 0.25$ as shown by Pfeuty [14]. Thus, the value of the index undergoes a non-analytic change at the boundary.

(2) In the floating phase, the correlation is non-oscillatory ($q = 0$) for $\kappa < 0.5$ and oscillatory ($q = \pi/2$)

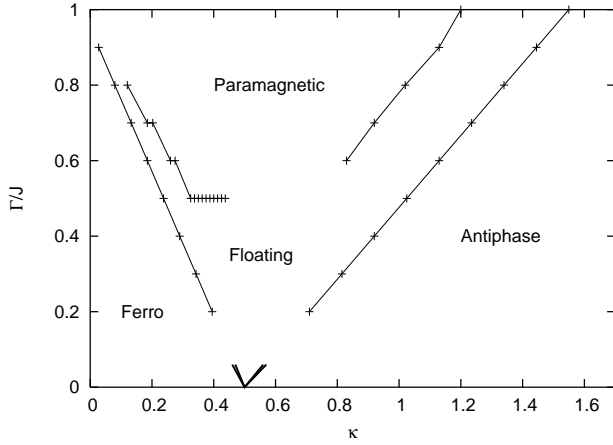


FIG. 5:

Phase diagram of the transverse ANNNI model as obtained from the first and the second perturbation scheme. The thick lines are exact results from the first perturbation scheme. The thin lines are approximate results from the second perturbation scheme. The thin line is not drawn in the region where the latter scheme becomes unreliable.

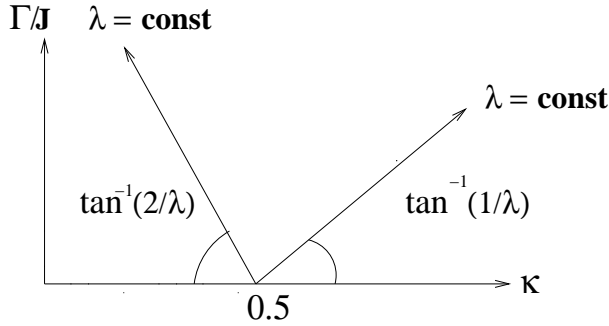


FIG. 6:

Plot of $\lambda = \text{constant}$ line with the κ axis.

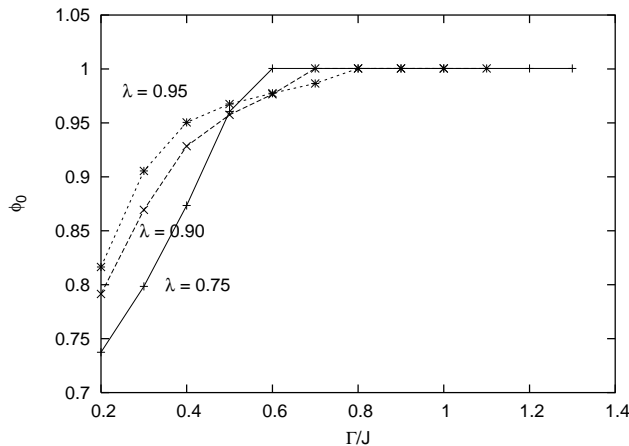


FIG. 7:

Plot of ϕ_0 vs. Γ for $\kappa < 0.5$. Here $\lambda = (1 - 2\kappa)J/\Gamma$.

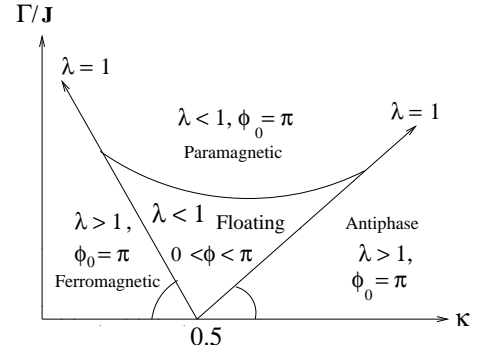


FIG. 8:

Schematic phase diagram showing the values of λ and ϕ_0 in different portions.

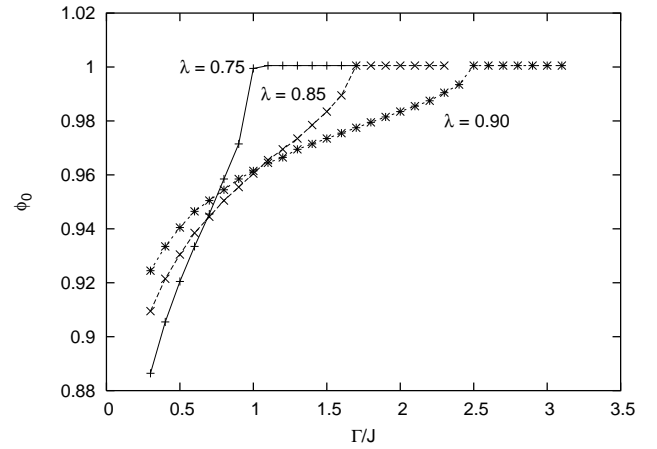


FIG. 9:

Plot of ϕ_0 vs. Γ for $\kappa > 0.5$. Here $\lambda = (\kappa - 0.5)J/\Gamma$

for $\kappa > 0.5$. Hence, the line $\kappa = 0.5$ is the “disorder line” [3] across which the modulation wavevector suffers a sudden change from 0 to $\pi/2$. We have also measured the perturbed energy $\langle h_0 \rangle + \langle h_1 \rangle$ and $\langle h'_0 \rangle + \langle h'_1 \rangle$ on two sides of the disorder line for a given Γ (Fig. 10). This energy remains continuous but suffers a change of slope at $\kappa = 0.5$. Since the first perturbation scheme does not indicate any phase transition around $\kappa = 0.5$, we guess that this change of slope is not the signature of any serious non-analytic behaviour but is only an outcome of the approximation inherent in perturbation calculation.

(3) Within the floating phase, for $\kappa > 0.5$, the nearest-neighbour correlation is zero (Eq. (28)) and the wave-vector is $q = \pi/2$, implying that the wave number $q/2\pi$ is equal to the number of domain walls per site. On the other hand, for $\kappa < 0.5$, the nearest-neighbour correlation is not at all zero (Fig. 11), but the correlation is non-oscillatory ($q = 0$), implying that the wave number $q/2\pi$ is *not* equal to the number of domain walls per site. One must note that (as mentioned above), the analytic treatments of Villain and Bak [9], and of Uimin and Rieger [4] assumes the equality of the wave-number

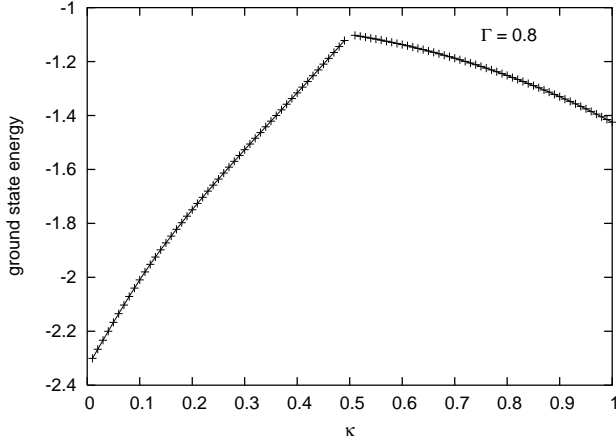


FIG. 10:

Plot of ground state energy vs. κ for $\Gamma = 0.8$

and the number of domain walls per site. This assumption thus agrees with our results for $\kappa > 0.5$ but not for $\kappa < 0.5$.

(4) The second perturbative scheme would be reliable only when the ratio $\langle h_1 \rangle / \langle h_0 \rangle$ or $\langle h'_1 \rangle / \langle h'_0 \rangle$ (accordingly as κ is < 0.5 or > 0.5) is small. We have included in Fig. 5 only those points where this ratio is less than some arbitrarily chosen number $1/3$. This criterion made us unable to locate the boundary between the paramagnetic and floating phase near $\kappa = 0.5$, $\Gamma = 0$ resulting in a gap there in Fig. 5. Some better approximation is needed to bridge this gap.

(5) The first and second perturbation schemes can be compared and reconciled in the following way. For the first perturbation scheme, the unperturbed Hamiltonian corresponds to the $\kappa = 0.5$, $\Gamma = 0$ point, and the exact expressions for the first order correction to energy gives exactly the directions along which the boundaries of ferromagnetic phase and antiphase emanate from this point (see Fig. 5). On the other hand, for the second perturbation scheme, the unperturbed Hamiltonian corresponds to the boundary lines of the ferromagnetic phase and the antiphase since on these lines $\langle h_1 \rangle$ and $\langle h'_1 \rangle$ are zero. The approximate estimate of the first order correction to energy gives the nature of the phase near the boundary. However, since the estimate is only approximate, at some regions of the parameter space, it is not reliable (as explained above).

Acknowledgments

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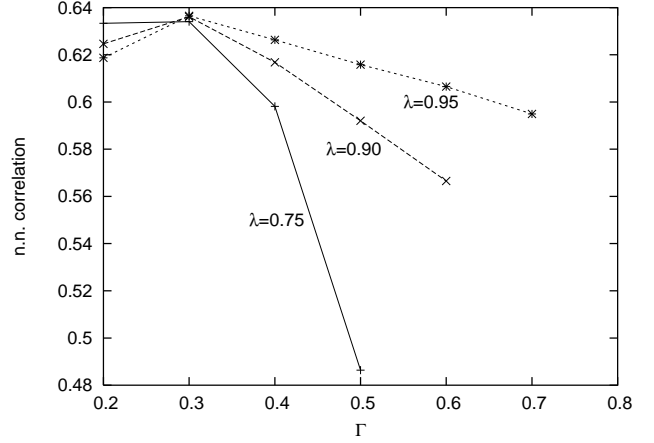


FIG. 11:

Plot of nearest neighbour correlation as a function of Γ for $\lambda=0.75, 0.90$ and 0.95

APPENDIX A HIGHER DERIVATIVES FOR THE FIRST ORDER PERTURBATION CORRECTION

We have derived earlier an expression

$$E^{(1)} = -N\Gamma \frac{2 \sin \phi_0 + 2\pi r - 3r\phi_0}{2\pi - \phi_0}$$

for the first order correction to the ground state energy of the Hamiltonian (see Eq. (3))

$$\mathcal{H}_{cl} = -J \sum_j [s_j^z s_{j+1}^z - \frac{1}{2} s_j^z s_{j+2}^z]$$

under perturbation by the Hamiltonian (see Eq. (4))

$$\mathcal{H}_p = \sum_j \Gamma [-s_j^x + r s_j^z s_{j+2}^z].$$

In this Appendix we shall show by the method of induction, that for all values of ϕ_0 in the range $0 < \phi_0 < \pi$, all higher derivatives of this quantity $E^{(1)}$ remain finite. For this purpose, we note that the first and second order derivatives are :

$$\frac{\partial E^{(1)}}{\partial r} = -N\Gamma \left(-\frac{4\pi}{(2\pi - \phi_0)} + 3 \right)$$

and

$$\frac{\partial^2 E^{(1)}}{\partial r^2} = -N\Gamma \left(\frac{8\pi^2}{(2\pi - \phi_0)^3 \sin \phi_0} \right).$$

Here we have used the equality

$$\frac{\partial \phi_0}{\partial r} = \frac{2\pi}{(2\pi - \phi_0) \sin \phi_0}$$

which can be obtained from Eq. (13). Thus, at least for $m = 1$ and 2 the derivatives can be expressed in the form

$$\frac{\partial^m E^{(1)}}{\partial r^m} = -N\Gamma \sum_{i=1}^{m'} k_i \frac{\cos^{\alpha_i} \phi_0}{(2\pi - \phi_0)^{\beta_i} \sin^{\gamma_i} \phi_0} \quad (29)$$

where $m' \sim 3^m$, and $\alpha_i, \beta_i, \gamma_i, k_i$ are constants ≥ 0 with the restriction $\gamma_i \leq \alpha_i$ (except for $m = 1$, where $\alpha_i = \gamma_i = 0$). Differentiating Eq.(29) once, it can be easily verified that the form (29) should be valid for $m + 1$ also, and is hence valid for all values of m . Since the right hand side of Eq. (29) diverges only when $\sin \phi_0$ vanishes, we conclude that so long as ϕ_0 is neither 0 or π the higher derivatives of $E^{(1)}$ remain finite.

APPENDIX B LONG RANGE CORRELATION FOR THE EXCITED STATES

Here we shall consider transverse Ising model with nearest neighbour interaction described by the Hamiltonian

$$\mathcal{H}^{TI} = - \sum_{j=1}^N [J s_j^z s_{j+1}^z + \Gamma s_j^x]. \quad (30)$$

The exact solution [2, 13, 14] for this Hamiltonian tells us that the 2^N number of energy eigenvalues are

$$E = 2\Gamma \sum_k \xi_k \Lambda_k \quad (31)$$

where $\Lambda_k = \sqrt{(\lambda^2 + 2\lambda \cos k + 1)}$, $\lambda = J/\Gamma$, ξ_k may be 0, ± 1 and k runs over $N/2$ equispaced values in the interval 0 to π .

In the text we have come across (more than once) ξ_k distribution of the following type :

$$\xi_k = \begin{cases} -1 & \text{for } k = 0 \text{ to } \phi \text{ (unexcited)} \\ 1 & \text{for } k = \phi \text{ to } \pi \text{ (excited)} \end{cases} \quad (32)$$

This is an excited state and reduces to the ground state only for $\phi = \pi$. This state is important for this work because it corresponds to the ground state after perturbation in the second perturbation scheme (Eq. (25)). It also corresponds to the first order correction in the first perturbation scheme (Eq. (11)). We shall present in this

Appendix the expressions for the longitudinal two-spin correlation function

$$C^z(n) \equiv \langle s_j^z s_{j+n}^z \rangle - \langle s_j^z \rangle^2 \quad (33)$$

(for $n \ll N$) in the long-range limit $n \rightarrow \infty$.

Let us consider the quantity,

$$\sigma^z(n) \equiv \langle s_j^z s_{j+n}^z \rangle \quad (34)$$

remembering that,

$$\lim_{n \rightarrow \infty} \sigma^z(n) = \langle s_j^z \rangle^2$$

Standard treatise [2, 13, 14] show that for $\phi = \pi$ (no excited state), this quantity is of the following form. For $\lambda > 1$,

$$\sigma^z(n) = \left(1 - \frac{1}{\lambda^2}\right)^{1/4} + A \exp(-\alpha n)$$

(A, α are constants depending on λ .) This corresponds to ferromagnetic state. For $\lambda < 1$,

$$\sigma^z(n) = A' \exp(-\alpha' n)$$

(A', α' are constants depending on λ .) This corresponds to paramagnetic state. There is a non-analyticity at the point $\lambda = 1$ where the second derivative of ground-state energy diverges.

Let us consider the correlation function $C^z(n)$ when $\lambda \neq 1$ and $0 < \phi < \pi$ (i.e. $\phi \neq 0$ and $\phi \neq \pi$ - some, but not all states are excited). We shall show elsewhere [18] that this quantity can be calculated exactly using Szego's Theorem. The results obtained are as follows. The quantity $\lim_{n \rightarrow \infty} \sigma^z(n)$ will be zero, so that $C^z(n)$ and $\sigma^z(n)$ are equal. Also, for $\lambda > 1$,

$$C^z(n) = \frac{0.590}{\sqrt{\sin \phi}} \left(1 - \frac{1}{\lambda^2}\right)^{1/4} \frac{\cos(\pi + \phi)n}{\sqrt{n}} \quad (35)$$

and for $\lambda < 1$,

$$C^z(n) = \frac{0.590 \sqrt{\sin \phi}}{\sqrt{(1 + \lambda^2 + 2\lambda \cos \phi)}} (1 - \lambda^2)^{1/4} \frac{1}{\sqrt{n}} \quad (36)$$

These expressions has been used in the text (Sec. IID, IIIB, IIIC) for the analysis of the phase diagram of 1D transverse ANNNI model.

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